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Spontaneous uptake of droplets into non-wetting capillaries

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ABSTRACT

In the present study, the spontaneous uptake of droplets into non-wetting capillaries was simulated by using many-body dissipative particle dynamics. The simulated results show that the droplets undergo a spontaneous uptake even for a non-wetting capillary. In contrast to the liquid in a reservoir in which the direction of liquid spontaneous movement in the capillary depends on the wettability, the moving direction of droplets in the capillary relies not only on the surface wettability but also the radius of the droplets. We give an explanation from the viewpoint of force balance. Our results demonstrate that capillary force could be used to drive liquid in microfluidics.

1. Introduction

Movement of liquids in capillaries has been being studied since last century as it plays an important role in many physical processes in nature [1,2]. In fact, many applications such as designing liquid droplet transportation devices in microfluidic systems [3,4] involve in liquid movement in micro- or nanotubes. However, the mechanism of spontaneous movement of liquids in capillaries is still a scientific challenge [5–10]. Most studies focus on the capillary imbibition and drainage of liquid from a reservoir, which usually could be modeled by considering the interaction between the capillary and the liquid reservoir. The movement direction of the liquid in a capillary depends on the wettability of the capillary itself. In 1988 Marmur [11] firstly studied the spontaneous uptake of droplets into non-wetting capillaries. He took the effects of droplet surface tension into consider and found that the Laplace pressure induced by the curvature of the droplets could drive the droplet to penetrate into the non-wetting capillaries. This novel phenomenon attracted much attention [12–18]. Hendy and coworkers studied liquid droplets penetrating into capillaries at nanoscopic level by using molecular dynamics. They established a model that can predict capillary absorption of non-wetting metal droplets by single-wall carbon nanotubes for the droplet radii below a critical size [12], and also proposed a modified Lucas-Washburn model which considers the finite radius of a droplet [13]. Besides above simulation and theoretical work, Willmott and coworkers performed experiments to demonstrate the spontaneous uptake of water droplets by non-wetting capillaries [14,15].

Although quite a number of investigations have been carried out to study the spontaneous uptake of droplets by non-wetting capillaries, it is still necessary to further explore its mechanism. In the present study, the capillary interaction between droplets with different radius and capillaries with different wettability was simulated by using many-body dissipative particle dynamics (MDPD). By designing a systematic simulation we aim at demonstrating that capillary force does play a key role for the uptake of droplets into non-wetting capillaries. Firstly, we obtain the relationship between the solid-liquid interaction parameter A_{sl} and static contact angle θ_s. Then we confirm that adopting this set of MDPD parameters, the liquid in a reservoir will be absorbed by the wetting capillaries and withdrawn when the contact angles are larger than 90°. With the same parameters, we studied the interaction between droplets with different radius and capillaries with different wettability. The paper is organized as follows. In Section 2, we give a brief introduction of the theoretical aspect about capillaries interacting with droplets. The details of MDPD are introduced in Section 3. We give our simulation results and discussion in Section 4 and conclusion in Section 5.

2. Theoretical background

It is well-known that when a capillary tube with internal radius R_t is brought into contact with liquid in a reservoir a meniscus of the liquid would form inside the capillary. If the capillary is hydrophilic, *i.e.* the contact angle on the capillary wall is smaller

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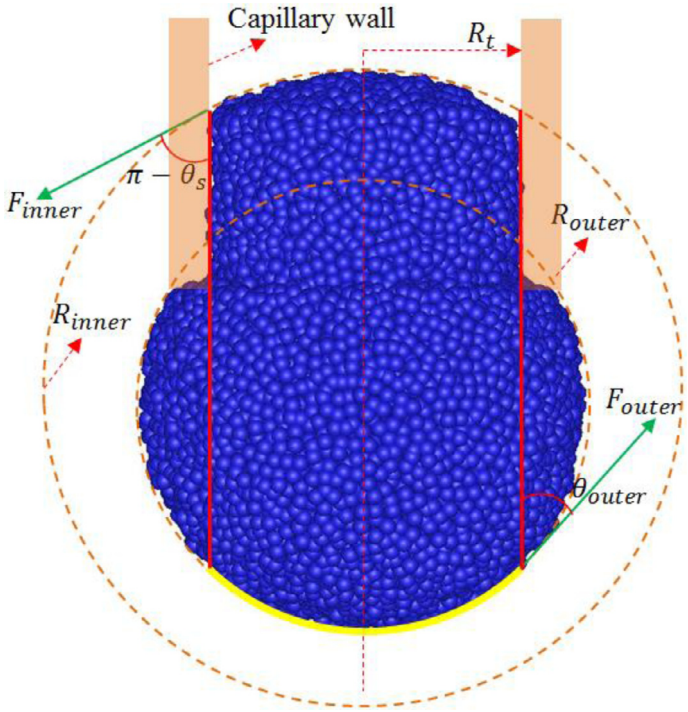

Fig. 1. Force balance explanation for capillary flow in a non-wetting capillary. The capillary wall is hidden.

than 90°, the meniscus would be concave and rise along the inner wall. On the contrary, if the capillary is hydrophobic, then a convex meniscus would form and the meniscus would move towards the opposite direction, hence the liquid would be withdrawn from the capillary. This phenomena can be explained from the point of view of force balance, hydrostatic pressure or energy transformation [19,20]. When replacing the reservoir by a droplet, an interesting thing would happen: the droplet may move upward along the hydrophobic capillary. This novel phenomenon can be explained by analysis of force balance for the droplet.

When the droplet is brought into contact with the non-wetting capillary, then a convex meniscus forms. The capillary force $F_{inner} = 2\pi R_t \cdot \gamma$ induced by liquid-gas surface tension γ will appear on the periphery $(2\pi R_t)$ of the meniscus and the vertical component $(F_{inner}\cos(\pi - \theta_s))$ can drive the liquid moving out from the capillary, as shown in Fig. 1. One part of the droplet surface, corresponding to yellow color in Fig. 1, also has a capillary force $F_{outer} = 2\pi R_t \cdot \gamma$ (*i.e.* $F_{outer} = F_{inner}$), and the vertical component of F_{outer} drive the liquid moving into the capillary. Forces acing on surfaces outside of the red solid lines are balanced in the vertical direction. When $R_{outer} < R_{inner}$, then $\theta_{outer} < \theta_s$, and we have $F_{outer}\cos\theta_{outer} > F_{inner}\cos(\pi - \theta_s)$. If we neglect the gravity, the net force exerting on the whole droplet will drive the liquid moving into the capillary. If the gravity is considered, the maximum displacement h can be obtained as follow:

$$\begin{aligned}\rho g h \cdot \pi {R_t}^2 &= F_{outer}\cos\theta_{outer} - F_{inner}\cos(\pi - \theta_s) \\ &= 2\pi R_t \cdot \gamma\left(\cos(\pi - \theta_s) + \frac{R_t}{R_d}\right) \\ h &= \frac{2\gamma\cos\theta_s}{\rho g R_t} + \frac{2\gamma}{\rho g R_d} \end{aligned} \quad (1)$$

Now, when $\theta_s > 90°$, the first term of the right-hand side of Eq. (1) is negative, but the sum of the right-hand side is not always negative. It is possible that the h will be positive and the droplet will penetrate into a non-wetting capillary spontaneously when R_d is small enough.

Table 1
Parameters adopted in the simulation (all in MDPD unit).

Name of parameter	Symbol of parameter	Value
Attractive coefficient	A	−80.0
Repulsive coefficient	B	25.0
Solid-liquid interaction parameter	A_{sl}	Tunable
Time step	ΔT	0.01
Temperature of the system	$K_B T$	1.0
Random coefficient	σ	1.0
Cutoff radius in $\omega^C(r_{ij})$	r_c	1.0
Cutoff radius in $\omega_d(r_{ij})$	r_d	0.75
Empirical velocity-Verlet coefficient	λ	0.65

When the droplet is replaced by a reservoir, *i.e.* $R_d \to \infty$, we get Eq. (2).

$$h = \frac{2\gamma\cos\theta_s}{\rho g R_t} \quad (2)$$

From Eq. (2) we know when $\theta_s < 90°$, $h > 0$, then the meniscus rises and *vice versa*.

3. Numerical method

MDPD [21,22] is a particle-based numerical method which has some similarities with molecular dynamics, but MDPD is a coarse-grained scheme. A MDPD particle is regarded as a cluster of molecules, and this makes it is suitable to simulate problems with larger scale in both time and space. Besides, for MDPD a van der Waals loop is added into the equation of state, which is essential to form free liquid/vapor interface in fluid systems. MDPD is widely used to study multiphase flow [23], droplet sliding [24] and capillarity [8,25], etc. Basically, the interaction between two adjacent MDPD particles consists of three parts–conservative force $\boldsymbol{F}_{ij}^{\boldsymbol{C}}$, dissipative force $\boldsymbol{F}_{ij}^{\boldsymbol{D}}$ and random force $\boldsymbol{F}_{ij}^{\boldsymbol{R}}$, see Eqs. (3–5):

$$\boldsymbol{F}_{\boldsymbol{ij}}^{\boldsymbol{C}} = A\omega^C(r_{ij})\boldsymbol{e}_{\boldsymbol{ij}} + B\left(\overline{\rho_i} + \overline{\rho_j}\right)\omega_d(r_{ij})\boldsymbol{e}_{\boldsymbol{ij}} \quad (3)$$

$$\boldsymbol{F}_{ij}^{D} = -\gamma\omega^D(r_{ij})\left(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{\boldsymbol{ij}}\right)\boldsymbol{e}_{ij} \quad (4)$$

$$\boldsymbol{F}_{ij}^{R} = \sigma\omega^R(r_{ij})\xi_{ij}\boldsymbol{e}_{ij} \quad (5)$$

$\omega^C(\mathrm{r_{ij}}) = 1 - \mathrm{r_{ij}}/\mathrm{r_c}$ and $\omega_\mathrm{d}(\mathrm{r_{ij}}) = 1 - \mathrm{r_{ij}}/\mathrm{r_d}$ are weight functions in Eq. (3). $\overline{\rho_i} = \sum_{\mathrm{i}\neq\mathrm{j}}\omega_\rho(\mathrm{r_{ij}})$ and $\omega_\rho(\mathrm{r_{ij}}) = \frac{15}{2\pi\,\mathrm{r_d}^3}(1 - \mathrm{r_{ij}}/\mathrm{r_d})^2$ calculate the local density in the many-body interaction. $\omega^D(r_{ij}) = \sqrt{1 - \mathrm{r_{ij}}/\mathrm{r_c}}$ and $\omega^R(r_{ij}) = \sqrt{\omega^D(r_{ij})}$ are weight functions in Eq. (4) and (5). Dissipative coefficient γ and random coefficient σ are coupled by $\sigma^2 = 2\gamma$ to stabilize the kinetic energy of the system. All the simulations were performed in a 3D system. The parameters adopted in this simulation are listed in Table 1.

4. Results and discussion

4.1. Wettability of droplet on capillary surfaces

To generate different wettability, the solid-liquid interaction parameter A_{sl} is tunable. A droplet is deposited on a flat and smooth substrate at a very gentle velocity $v = 0.1$ and in all simulations we neglect the effect of gravity. When the droplet is in equilibrium, a stable partial sphere could be obtained and then we can calculate the static contact angle θ_s, as shown in Fig. 2. The calculation method of contact angle can be found in our previous work [26,27]. Fig. 3 shows the relationship between A_{sl} and θ_s. Here, we test droplets with three different sizes to find out if the wettability is dependent on droplet size. As shown in Fig. 3, the wettability